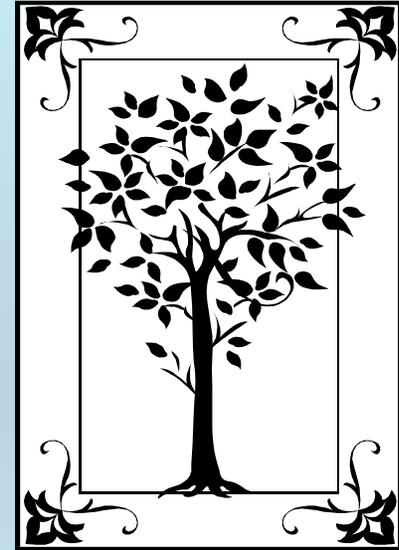


**METADATA AND NUMERICAL DATA CAPTURE:
Temperature and Pressure of
Liquid-Liquid-Vapor Equilibrium**

**Guided Data
Capture (GDC)**



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE
**Temperature and Pressure of
Liquid-Liquid-Vapor (L_1L_2V) Equilibrium**
with the Guided Data Capture (GDC) software.

NOTE:

The tutorials proceed sequentially to ease the descriptions. **It is not necessary to enter *all* compounds before entering *all* samples, etc.**

Compounds, samples, properties, etc., can be added or modified at any time.

However, the hierarchy must be maintained (i.e., a property cannot be entered, if there is no associated sample or compound.)

The experimental data used in this example is from:

Fluid Phase Equilibria of Binary n-Alkane + Squalane Systems

Diana E. Nanu¹, Wim Poot¹, Dan Geană², Theodoor W. de Loos^{1*}

¹Delft University of Technology, Department of Chemical Technology, Laboratory of Applied Thermodynamics and Phase Equilibria, Julianalaan 136, 2628 BL Delft, The Netherlands

²University “Politehnica” Bucharest, Department of Applied Physical Chemistry and Electrochemistry, Spl. Independentei 313, 78126 Bucharest, Romania

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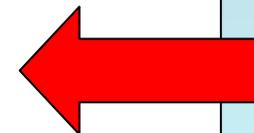
Temperature and Pressure of Liquid-Liquid-Vapor (L_1L_2V) Equilibrium for (ethane + squalane)

Table 2. Experimental Data of the Three-Phase Equilibrium L_1L_2V in the Ethane-Squalane System

T/K	p/MPa
295.57	3.930 ^a
295.71	3.961
296.00	3.979
296.53	4.028
297.38	4.105
297.89	4.166
298.30	4.196
298.79	4.231
299.33	4.287
300.34	4.374
300.94	4.436
301.35	4.474
302.37	4.570
302.53	4.581
303.43	4.685
304.42	4.775
305.32	4.865
306.51	4.996
306.69	5.013 ^b

^a LCEP ($L_2 = L_1 + V$). ^b UCEP ($L_2 + L_1 = V$).

**This data
set is
considered
here.**



Guided Data Capture - Thermophysical and Thermochemical Data

File Edit Tools Help

Reference Compound Sample Mixture Reaction **Property** Data Tables

2002 nan poo 1

- ethane
 - Sample 1 (cm,99.95m%,nc:)
- propane
 - Sample 1 (cm,99.95m%,nc:)
- squalane
 - Sample 1 (cm,99m%,glc:)
- ethane + squalane**
 - z. file, 1 (set 1), 0 Method:VISOB5 dt=0.02 dP=5
- propane + squalane

2. CLICK *Property*

1. SELECT the *mixture* for which the data are to be captured.

NOTE: The **bibliographic information, compound identities, sample descriptions, and mixture** were entered previously. (There are separate tutorials, which describe capture of this information, if needed.)

Property and experimental method for ethane + squalane

Help

Property group: Vapor pressure; Boiling temperature; and Azeotropic T & P

Property: Vapor or Sublimation pressure

Units: MegaPa

Method of measurement:

Experimental purpose:

Comment (optional)

OK Cancel

1. SELECT the **Property Group:** *Vapor pressure, etc.* from the menu. Here, the transition is between 1 and 2 liquid phases.

2. SELECT the **Property:** *Vapor or Sublimation pressure* from the menu.

3. SELECT the **Units;** *MPa* here.

Property and experimental method for ethane + squalane

Help

Property:

Property:

Units:

1. SELECT Method of Measurement from the list.

NOTE: *Other* is a valid selection and should include a brief description in the **Comment** field, such as shown below.

Method of measurement: Other experimental method (please, describe in "Comments")

Experimental purpose: Principal objective of the work

2. SELECT the Experimental Purpose
from the list provided.

Comment
(optional)

Cailletet apparatus according to the synthetic method. See details in de Loos et al, J. Chem. Eng. Data, 1986, 31, 166.

3. CLICK *OK*

OK

Cancel

SELECTION of # of Phases in Equilibrium and # of Constraints

Vapor or Sublimation pressure (MegaPa) as function of 1 variable(s)

Mixture: ethane + squalane

Phases in equilibrium: 3

Constraints: 0

Independent variables: 1

Phase of the Property Value(s)

Enter the # of **Phases in equilibrium**.

There are **3** phases (L_1, L_2, V) in equilibrium.

Enter the # of **Constraints**.

There are **0** constraints (such as T, p , or x) in the example.

Vapor or Sublimation pressure (MegaPa) as function of 1 variable(s)

Mixture: ethane + squalane

Phases in equilibrium: 3 Constraints: 0 Independent variables: 1 Property set #: **Sample # 1** **Sample # 1**

Phase of the Property Value(s): Precision of the Property Value(s): MegaPa %

Definition of Measurement Results (Absolute vs Relative):

Data presentation: Experimental values

Comments (Optional): Cailletet apparatus according to the synthetic method. See details in de Loos et al, J. Chem. Eng. Data, 1986, 31, 166.

Property and method Numerical Data Cancel



Multiple Samples for a given component can be accommodated, but this is rarely needed.

Select phases

Vapor or Sublimation pressure (MegaPa) as function of 1 variable(s)

Mixture: ethane + squalane

Phases in equilibrium: 3 Constraints: 0 Independent variables: 1

Phase of the Property Value(s) Liquid mixture 1

Phase 2
Liquid mixture 2

Phase 3
Gas

1) SELECT *Liquid Mixture 1* from the list provided for the **Phase of the Property Value**

2. SELECT *Liquid Mixture 2* for **Phase 2**

3. SELECT *Gas* for **Phase 3**

Specification of constraints, constraint values, and constraint units

Vapor or Sublimation pressure (MegaPa) as function of 1 variable(s)

Mixture: ethane + squalane

Phases in equilibrium: 3 Constraints: 0 Independent variables: 1 Property set #: 1 Sample #: 1 Sample #: 1

Phase of the Property Value(s): Liquid mixture 1 Precision of the Property Value(s): MegaPa %

Phase 2: Liquid mixture 2

Phase 3: Gas

Independent variable 1: Temperature Units: K Uncertainty: %

Definition of Measurement Results (Absolute vs Relative):

Property and method:

os et al, J. Chem. Eng. Data, 1986, 31, 166.

Numerical Data Cancel

1. SELECT the the Independent Variable (*T* here) from the menu.

2. SELECT Units for the Variable(s). Include estimated Uncertainty, if known.

Measurement definition and Data presentation

1. SELECT *Direct Value* (as compared with Relative Value) from the list defining the **Measurement Results**

2. SELECT the appropriate **Data presentation method. *Experimental values* here.**

3. CLICK *Numerical Data*

Mixture: ethane + squalane
Phases in equilibrium: 3 Constraints: 0 Independent variable
Phase of the Property Value(s) Liquid mixture 1
Phase 2 Liquid mixture 2
Phase 3 Gas
Independent variable 1 Temperature of Liquid mixture 1 Units: K Uncertainty: %
Definition of Measurement Results (Absolute vs Relative) Direct value
Data presentation Experimental values
Comments (Optional): Cailletet apparatus according to the synthetic method. See details in de Loos et al, J. Chem. Eng. Data, 1986, 31, 166.
Property and method Numerical Data Cancel

Vapor or Sublimation pressure (MegaPa) as function of 1 variable(s)

File Edit Action Help

	Var 1	Property
1		

TYPE, or much preferably, PASTE the variable and property values into the table.

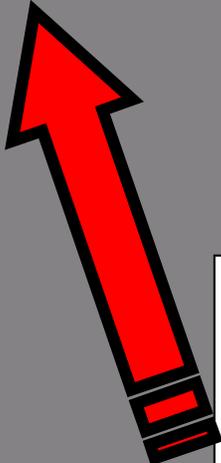


Table 2. Experimental Data of the Three-Phase Equilibrium L_1L_2V in the Ethane-Squalane System

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305.32	4.865
306.51	4.996
306.69	5.013 ^b

^a LCEP ($L_2 = L_1 + V$). ^b UCEP ($L_2 + L_1 = V$).

Vapor or Sublimation pressure (MegaPa) as function of 1 variable(s)

File Edit Action Help

	Var 1	Property
1	295.57	3.930
2	295.71	3.961
3	296.00	3.979
4	296.53	4.028
5	297.38	4.105
6	297.89	4.166
7	298.30	4.196
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15	303.43	4.685
16	304.42	4.775
17	305.32	4.865
18	306.51	4.996
19	306.69	5.013

Clear the Table

Table 2. Experimental Data of the Three-Phase Equilibrium L_1L_2V in the Ethane-Squalane System

<i>T</i> /K	<i>p</i> /MPa
295.57	3.930 ^a
295.71	3.961
296.00	3.979
296.53	4.028
297.38	4.105
297.89	4.166
298.30	4.196
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305.32	4.865
306.51	4.996
306.69	5.013 ^b

^a LCEP ($L_2 = L_1 + V$). ^b UCEP ($L_2 + L_1 = V$).

NOTE: Simple CUT/PASTE procedures can be used within the table to convert the original table into the required number of columns. (This can also be done externally in spreadsheet software, e.g., EXCEL.)

Vapor or Sublimation pressure (MegaPa) as function of 1 variable(s)

File Edit Action Help

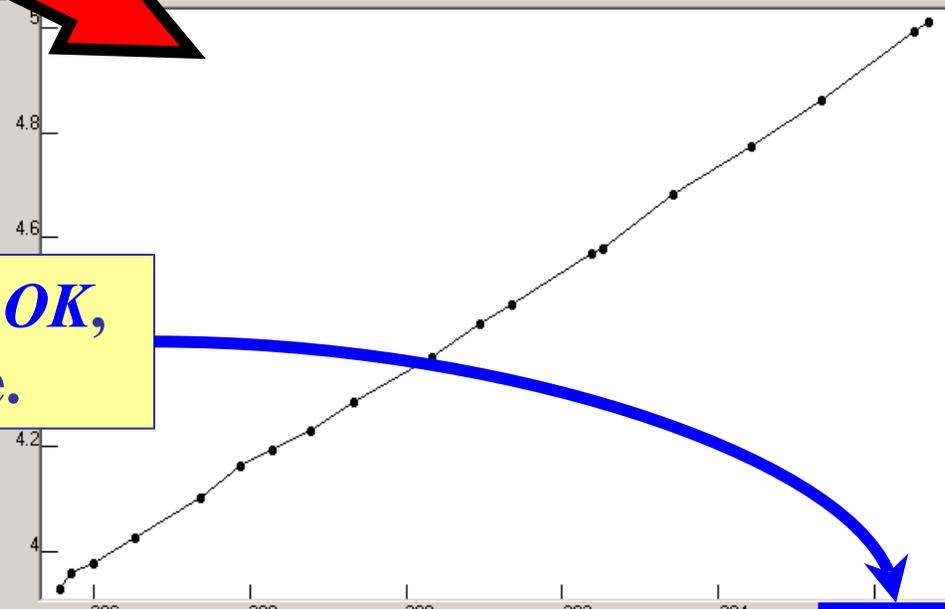
	Var 1	Property
1	295.57	3.930
2	295.71	3.961
3	296.00	3.979
4	296.53	4.028
5	297.38	4.105
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16	304.42	4.775
17	305.32	4.865
18	306.51	4.996
19	306.69	5.013

1. CLICK *View plot* to see a plot and check for typographical errors.

Clear the Table

View plot

Vapor or Sublimation pressure as function of Temperature



2. CLICK *OK*, when done.

X = Var 1

ln Y vs 1/X

OK

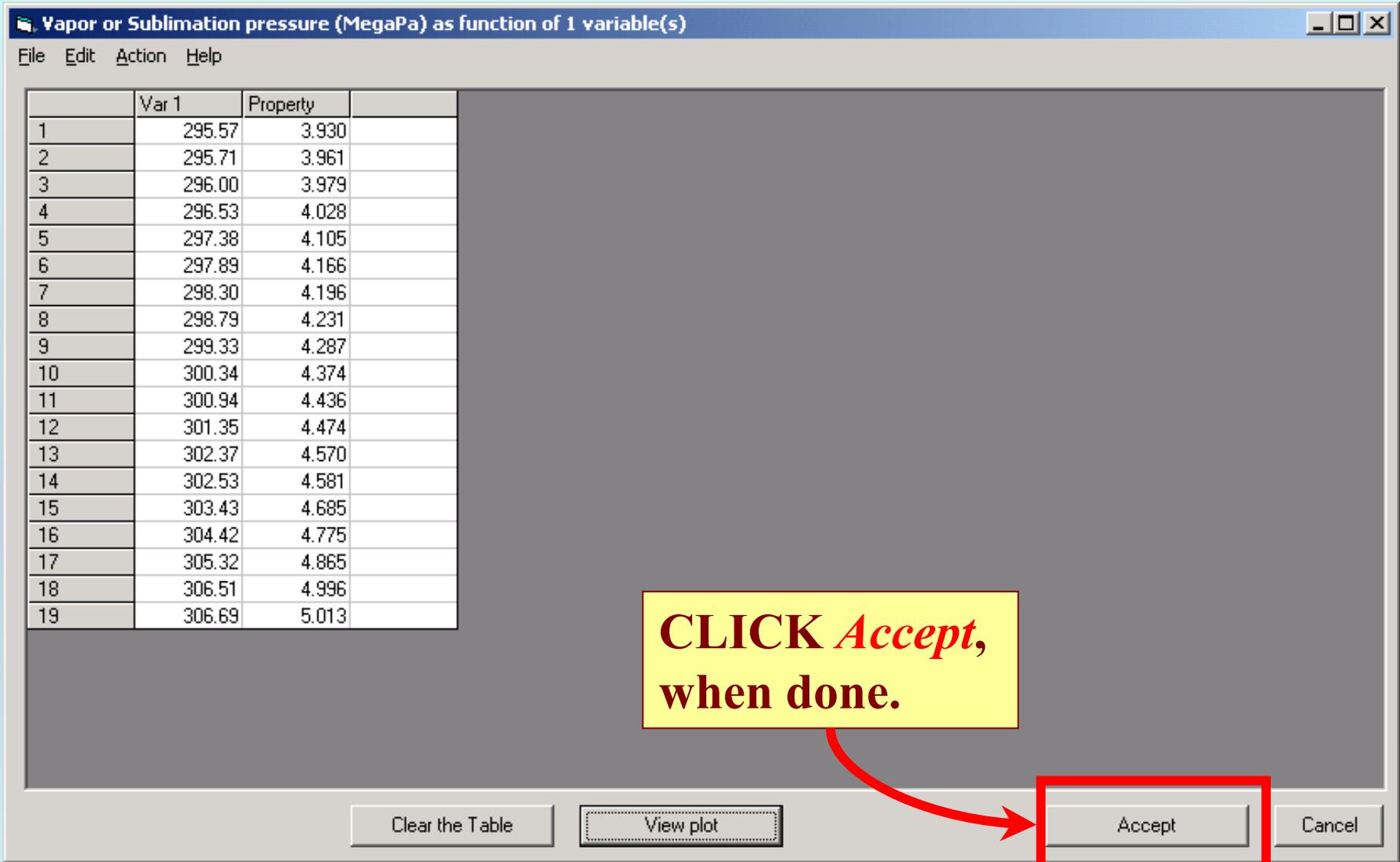
Vapor or Sublimation pressure (MegaPa) as function of 1 variable(s)

File Edit Action Help

	Var 1	Property
1	295.57	3.930
2	295.71	3.961
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4	296.53	4.028
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17	305.32	4.865
18	306.51	4.996
19	306.69	5.013

**CLICK *Accept*,
when done.**

Clear the Table View plot **Accept** Cancel

The image shows a software window titled "Vapor or Sublimation pressure (MegaPa) as function of 1 variable(s)". The window has a menu bar with "File", "Edit", "Action", and "Help". On the left side, there is a table with two columns: "Var 1" and "Property". The table contains 19 rows of data. On the right side, there is a large gray area, likely a plot area. At the bottom of the window, there are four buttons: "Clear the Table", "View plot", "Accept", and "Cancel". The "Accept" button is highlighted with a red rectangular box. A yellow callout box with a red border and a red arrow pointing to the "Accept" button contains the text "CLICK *Accept*, when done."

Guided Data Capture - Thermophysical and Thermochemical Data

File Edit Tools Help

Reference

Compound

Sample

Mixture

Reaction

Property

Data Tables

2002 nan poo 1

ethane

Sample 1 (cm,99.95m%,nc;)

propane

Sample 1 (cm,99.95m%,nc;)

squalane

Sample 1 (cm,99m%,glc;)

ethane + squalane

^2: Ile, T (Set 1), B Method:VIS OBS dT=0.02 dP=5

^1: Ile, P (Set 1), B Method:OTHER dP=0.005 dT=0.02

propane + squalane

NOTE: The new data set now appears in the tree under the appropriate *mixture*.

NOTE: DOUBLE CLICKING on the *data set* allows editing of all entered information.

END

**Continue with other compounds,
samples, properties, reactions, etc...**

or save your file and exit the program.